LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030718\
Data File : BF103499.D
Acq On : 7 Mar 2018 14:28
Operator : SJ/JU
Sample : J1699-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B5

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	4	9	16	rVB	223778	315701	10.21%	1.070%
2	5.104	510	513	527	rBV	54068	89247	2.89%	0.303%
3	5.493	575	579	608	rBV	2083573	3093365	100.00%	10.486%
4	6.504	747	751	769	rBV	1988635	2995880	96.85%	10.155%
5	6.634	769	773	786	rVV	2636465	2899793	93.74%	9.829%
6	6.863	809	812	828	rBV	782979	868449	28.07%	2.944%
7	7.016	834	838	857	rBV	2075005	2306555	74.56%	7.819%
8	7.434	905	909	933	rBV	1466005	2121101	68.57%	7.190%
9	8.145	1027	1030	1049	rBV	881953	1257590	40.65%	4.263%
10	9.022	1174	1179	1182	rBV	25937	34069	1.10%	0.115%
11	9.086	1186	1190	1199	rVB	154645	171581	5.55%	0.582%
12	9.222	1206	1213	1223	rBV	2849828	3089880	99.89%	10.474%
13	9.328	1228	1231	1236	rVV4	26641	38310	1.24%	0.130%
14	9.398	1240	1243	1255	rVB3	22167	45215	1.46%	0.153%
15	9.904	1325	1329	1342	rBV	1107056	1211511	39.16%	4.107%
16	10.292	1391	1395	1397	rBV	70163	55753	1.80%	0.189%
17	10.316	1397	1399	1402	rVB	63125	51254	1.66%	0.174%
18	10.704	1461	1465	1477	rBV	1293580	1619002	52.34%	5.488%
19	10.792	1477	1480	1486	rVB2	47218	59787	1.93%	0.203%
20	10.898	1493	1498	1501	rBV	35730	38397	1.24%	0.130%
21	11.239	1553	1556	1559	rBV	38166	37852	1.22%	0.128%
22	11.333	1569	1572	1575	rBV3	36649	35309	1.14%	0.120%
23	11.398	1580	1583	1592	rBV	941752	1114222	36.02%	3.777%
24	11.545	1605	1608	1612	rBV	113411	91783	2.97%	0.311%
25	11.669	1626	1629	1631	rBV	42761	40692	1.32%	0.138%
26	11.769	1643	1646	1650	rBV	275828	230511	7.45%	0.781%
27	11.910	1668	1670	1672	rBV3	35709	33997	1.10%	0.115%
28	11.945	1673	1676	1681	rVB	391140	323091	10.44%	1.095%
29	12.075	1696	1698	1701	rVB	42173	32792	1.06%	0.111%
30	12.457	1760	1763	1765	rBV2	458821	466401	15.08%	1.581%
31	12.480	1765	1767	1777	rVV	663621	686726	22.20%	2.328%
32	12.563	1778	1781	1786	rVB	158241	140548	4.54%	0.476%
33	12.780	1815	1818	1821	rVB3	36524	32069	1.04%	0.109%
34	12.839	1825	1828	1831	rBV	79874	78268	2.53%	0.265%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030718\
Data File : BF103499.D
Acq On : 7 Mar 2018 14:28
Operator : SJ/JU
Sample : J1699-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B5

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.986	1848	1853	1860	rBV	1937575	1932502	62.47%	6.551%
36	13.192	1883	1888	1891	rBV	99049	101355	3.28%	0.344%
37	13.539	1943	1947	1951	rVB	78602	82643	2.67%	0.280%
38	13.863	1999	2002	2008	rBV	135725	164218	5.31%	0.557%
39	14.004	2023	2026	2029	rVB	42144	37191	1.20%	0.126%
40	14.057	2031	2035	2043	rBV	623411	723593	23.39%	2.453%
41	14.498	2107	2110	2113	rBV3	29513	41463	1.34%	0.141%
42	15.145	2217	2220	2223	rVB	38872	41525	1.34%	0.141%
43	15.568	2287	2292	2303	rVB	388907	612739	19.81%	2.077%
44	15.974	2357	2361	2365	rVB2	39023	57129	1.85%	0.194%

Sum of corrected areas: 29501059

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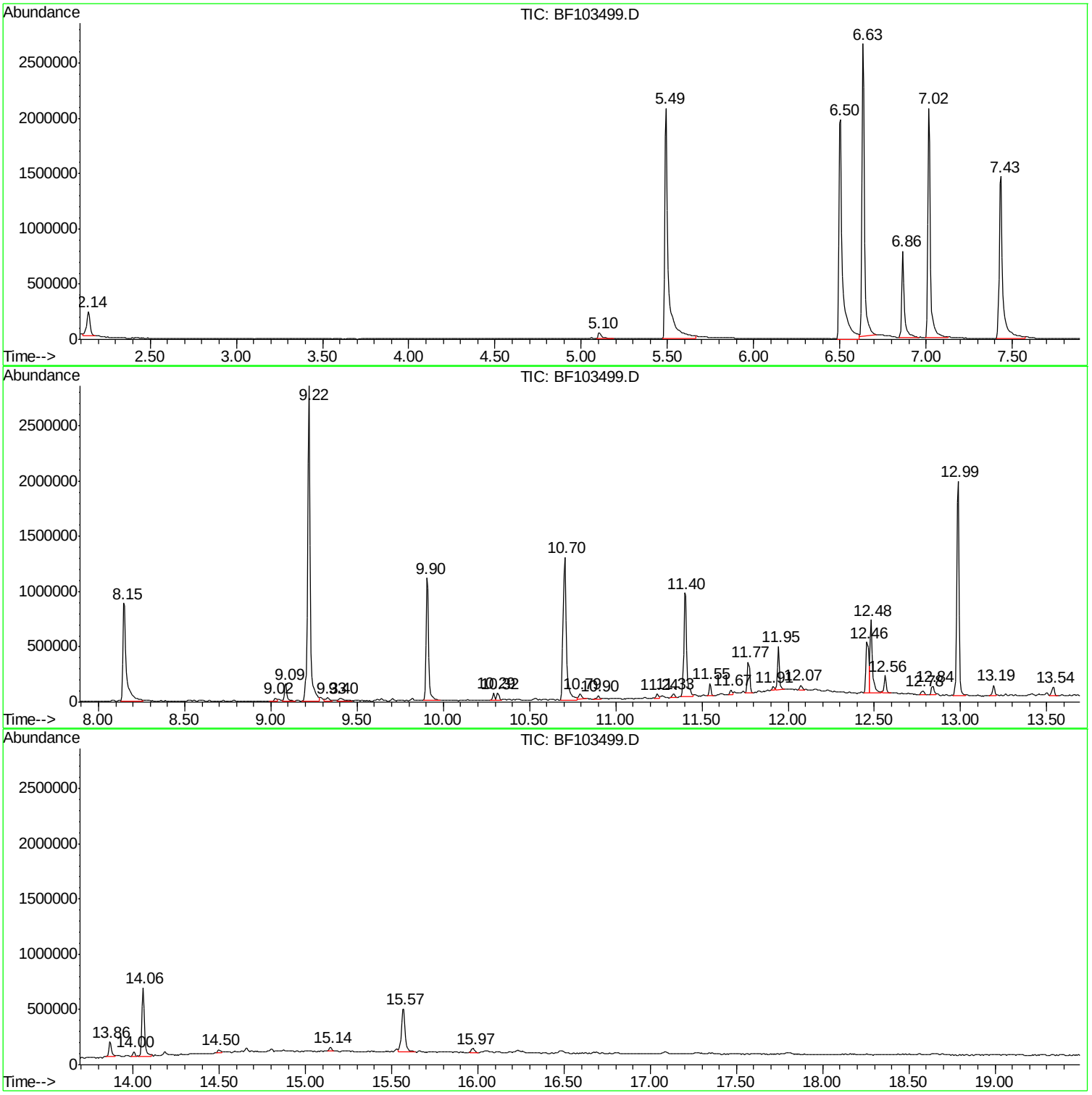
Instrument : BNA_F
ClientSampleId : B5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Data File : BF103499.D
Acq On : 7 Mar 2018 14:28
Operator : SJ/JU
Sample : J1699-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

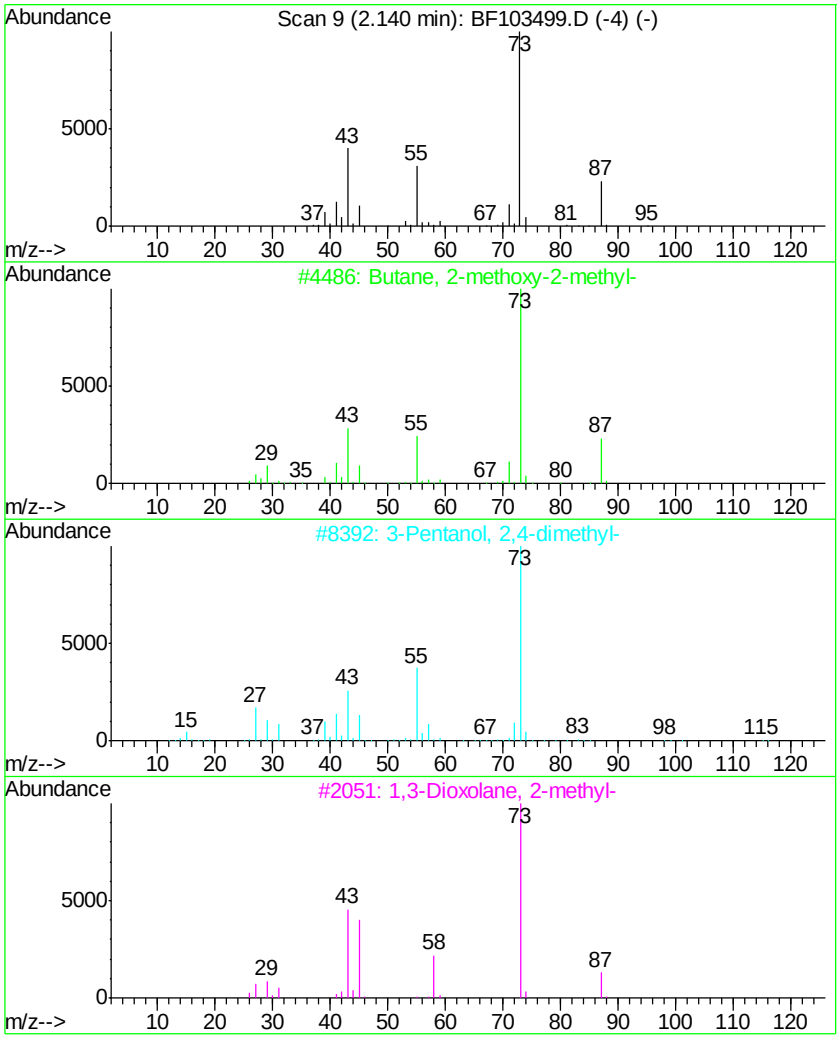
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

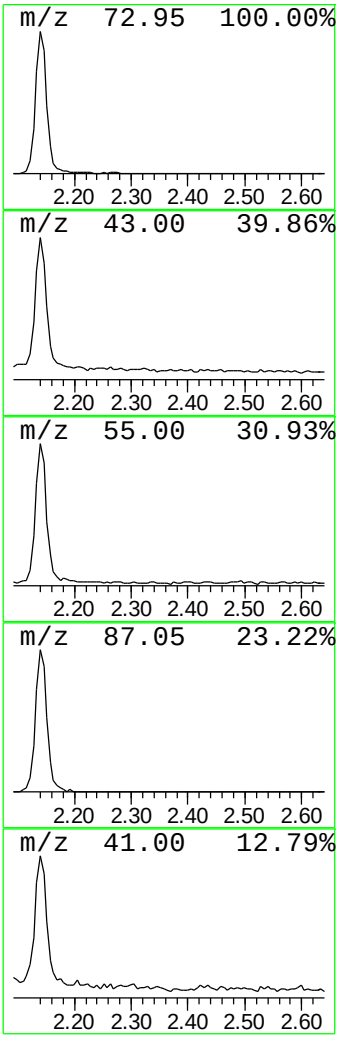
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	7.27 ng	315701	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	32
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





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Sample : J1699-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B5

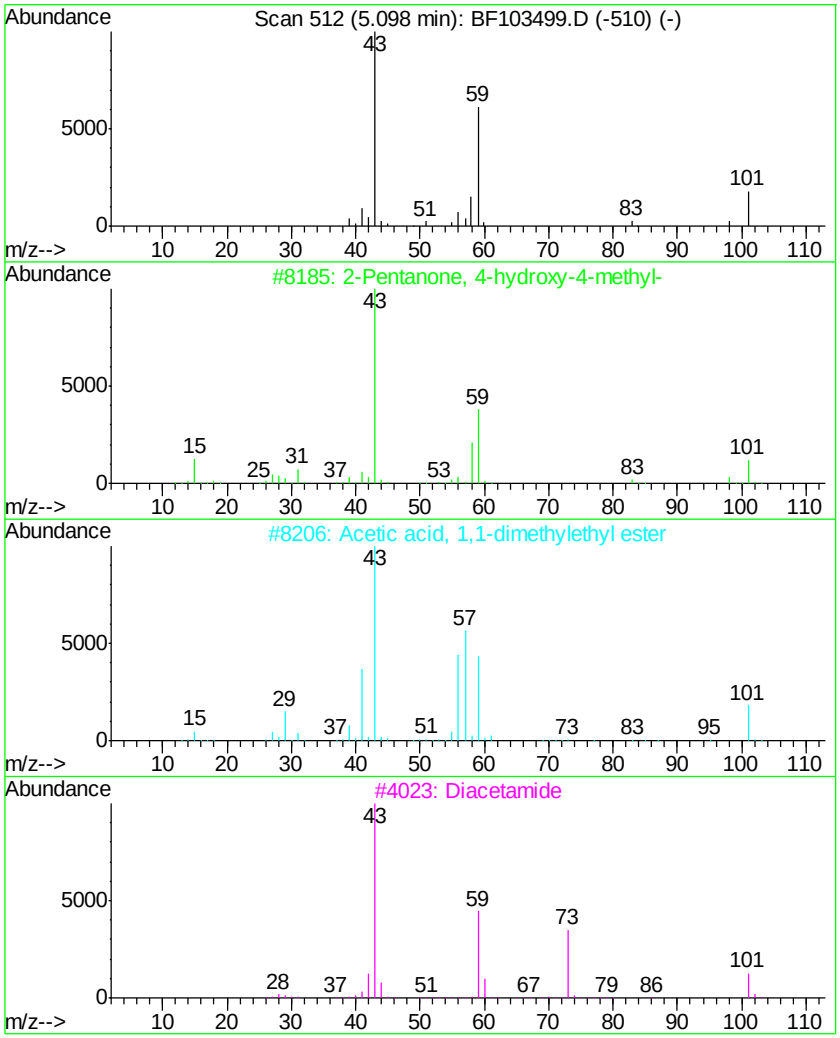
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

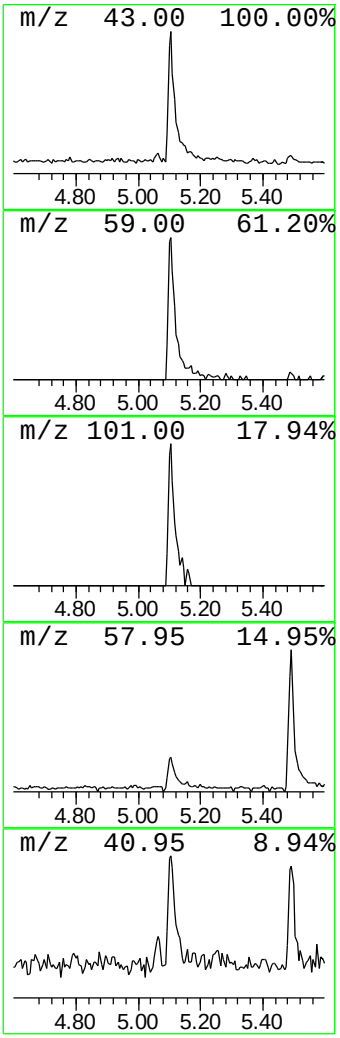
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	2.06 ng	89247	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Diacetamide	101	C4H7NO2	000625-77-4	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	1,2-Butanediol	90	C4H10O2	000584-03-2	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030718\
Data File : BF103499.D
Acq On : 7 Mar 2018 14:28
Operator : SJ/JU
Sample : J1699-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

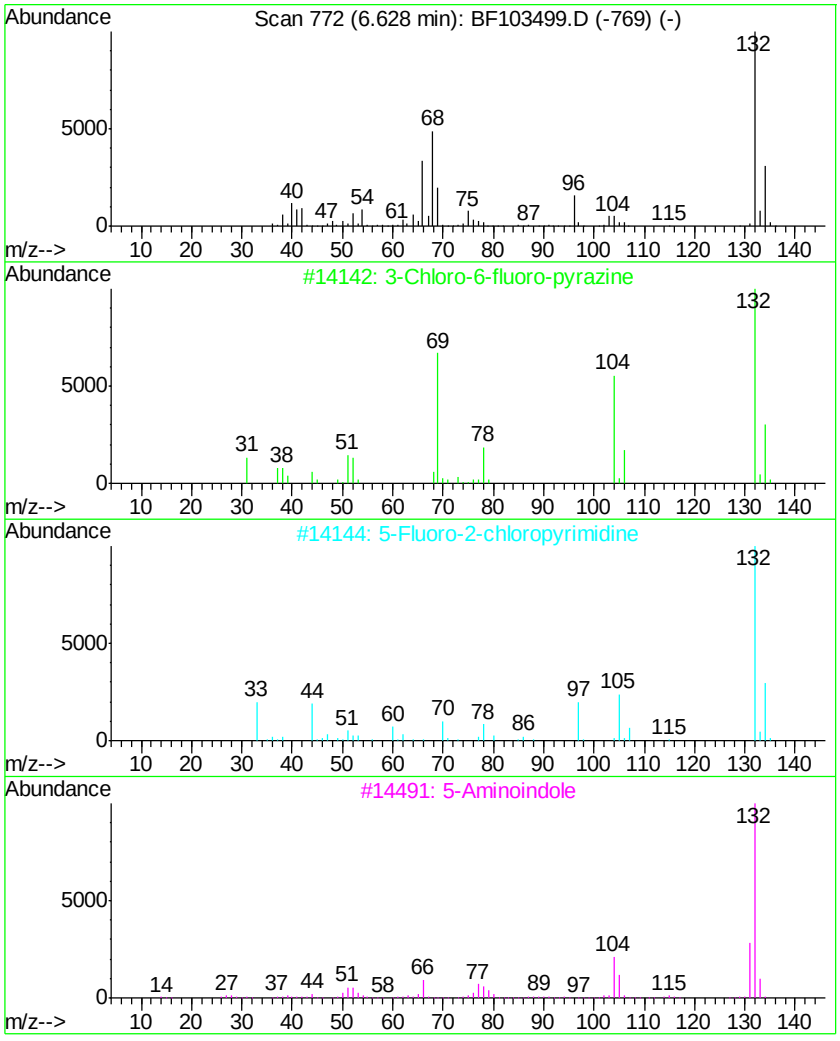
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

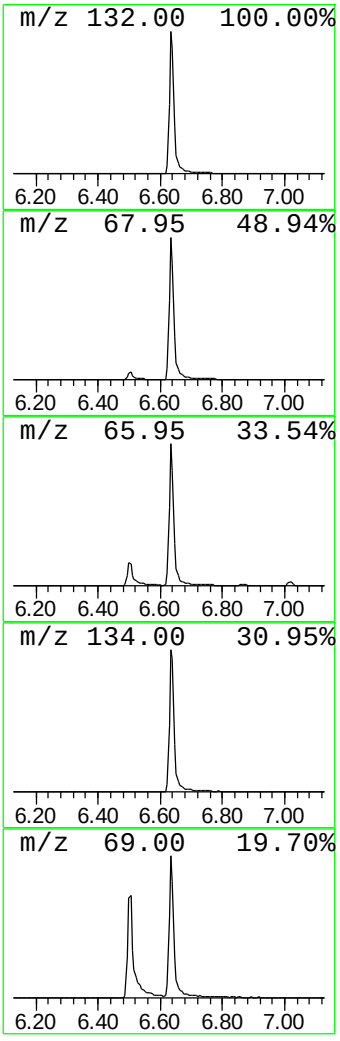
****

Peak Number 3 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	66.78 ng	2899790	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
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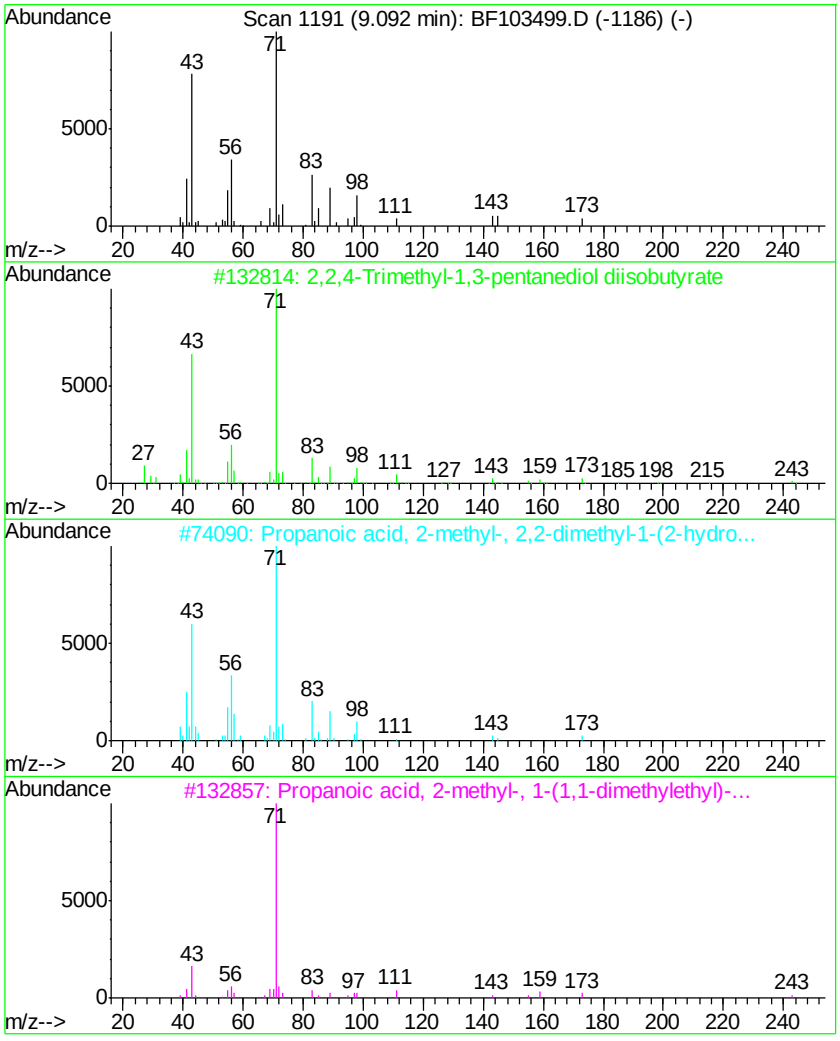
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

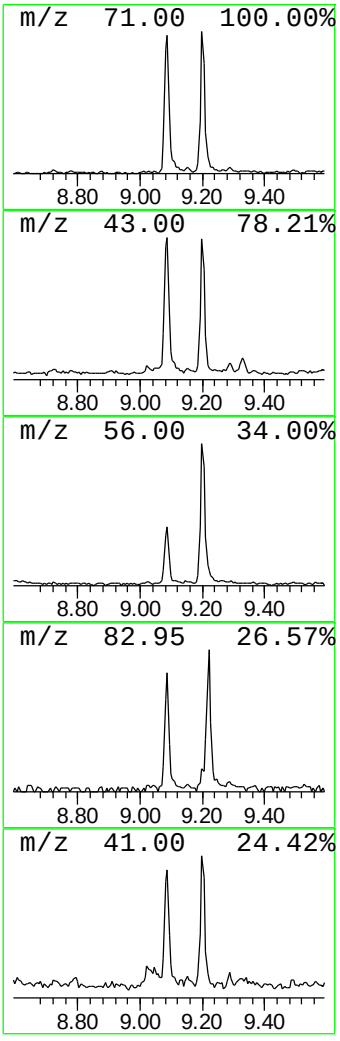
****

Peak Number 5 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.09	2.83 ng	171581	Acenaphthene-d10	9.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	78
2	Propanoic acid, 2-methyl-, 2,2-d...	216	C12H24O3	074367-33-2	74
3	Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	50
4	3-Hexanone, 2,5-dimethyl-4-nitro-	173	C8H15NO3	059906-54-6	43
5	2,5-Dimethyl-1,5-hexadien-3-ol	126	C8H14O	017123-63-6	38





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Instrument : BNA_F
ClientSampleId : B5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

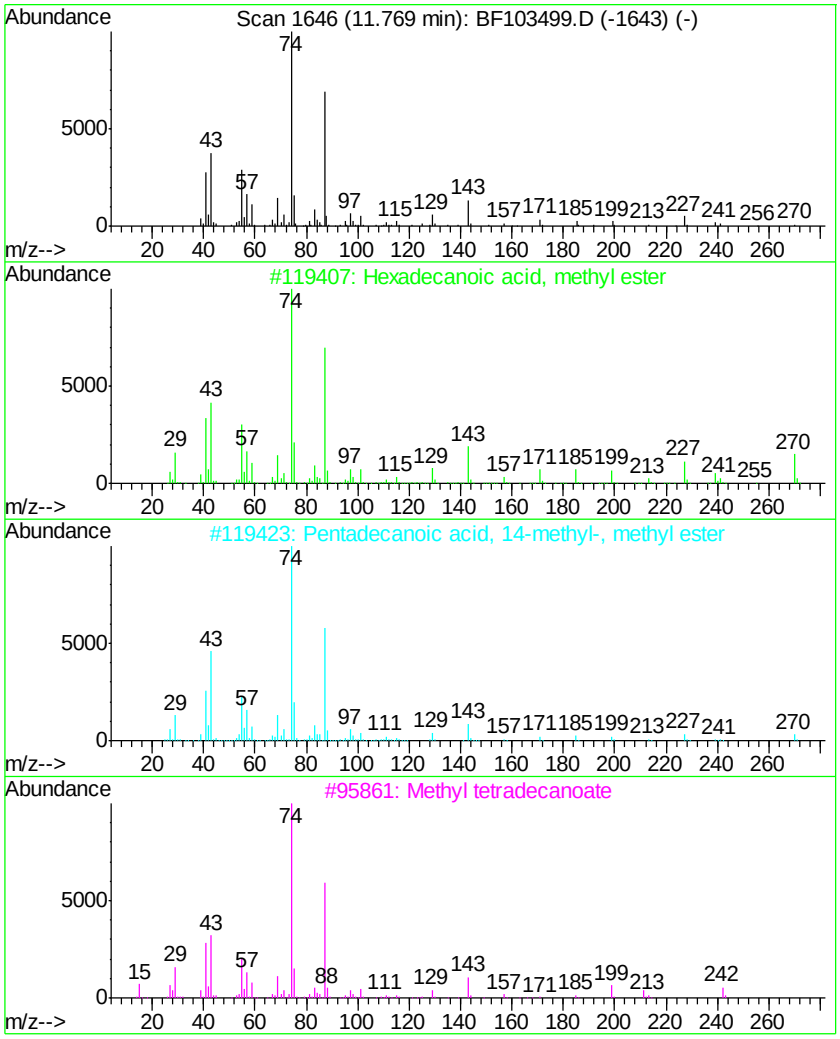
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

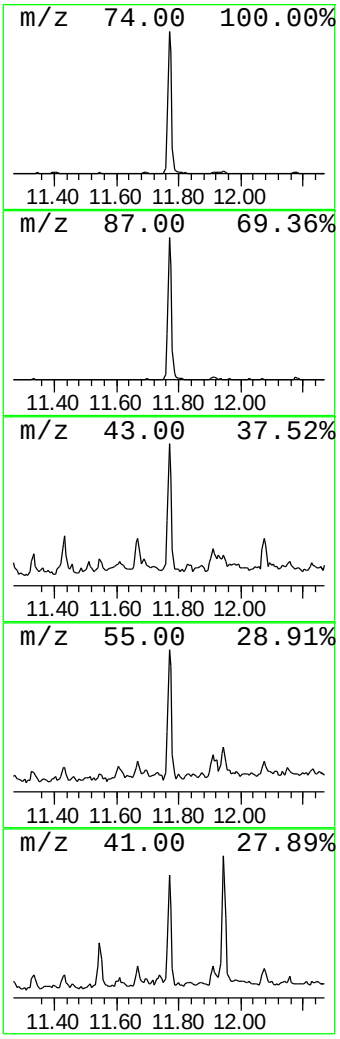
****

Peak Number 6 Hexadecanoic acid, methyl e... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.77	4.14 ng	230511	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	90
4	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	90
5	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	90





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Sample : J1699-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

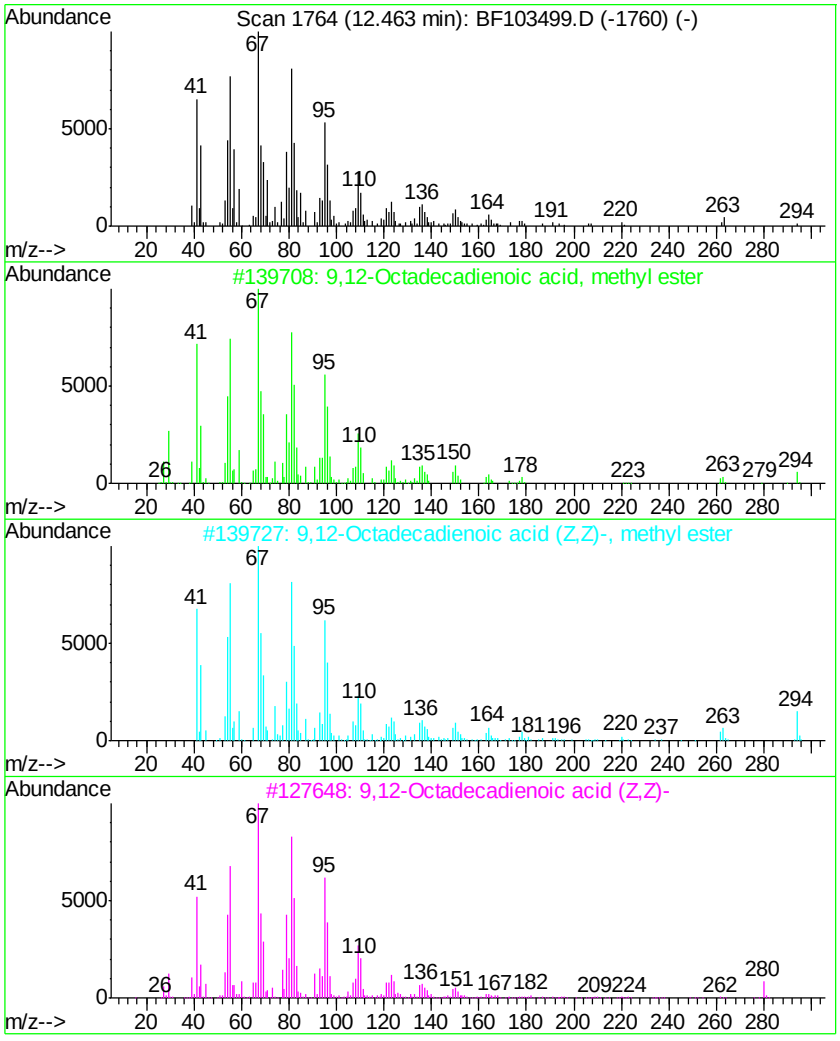
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

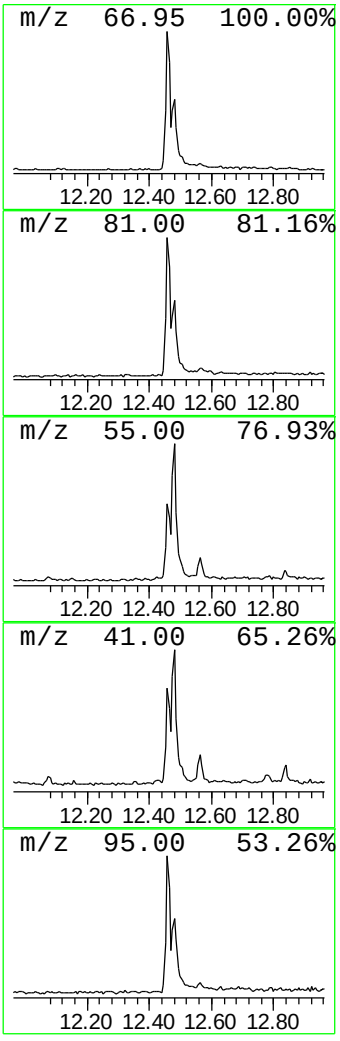
****

Peak Number 7 9,12-Octadecadienoic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.46	8.37 ng	466401	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
3	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95
4	2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	94
5	11,14-Octadecadienoic acid, meth...	294	C19H34O2	056554-61-1	91





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Sample : J1699-13
Misc :
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Instrument : BNA_F
ClientSampleId : B5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

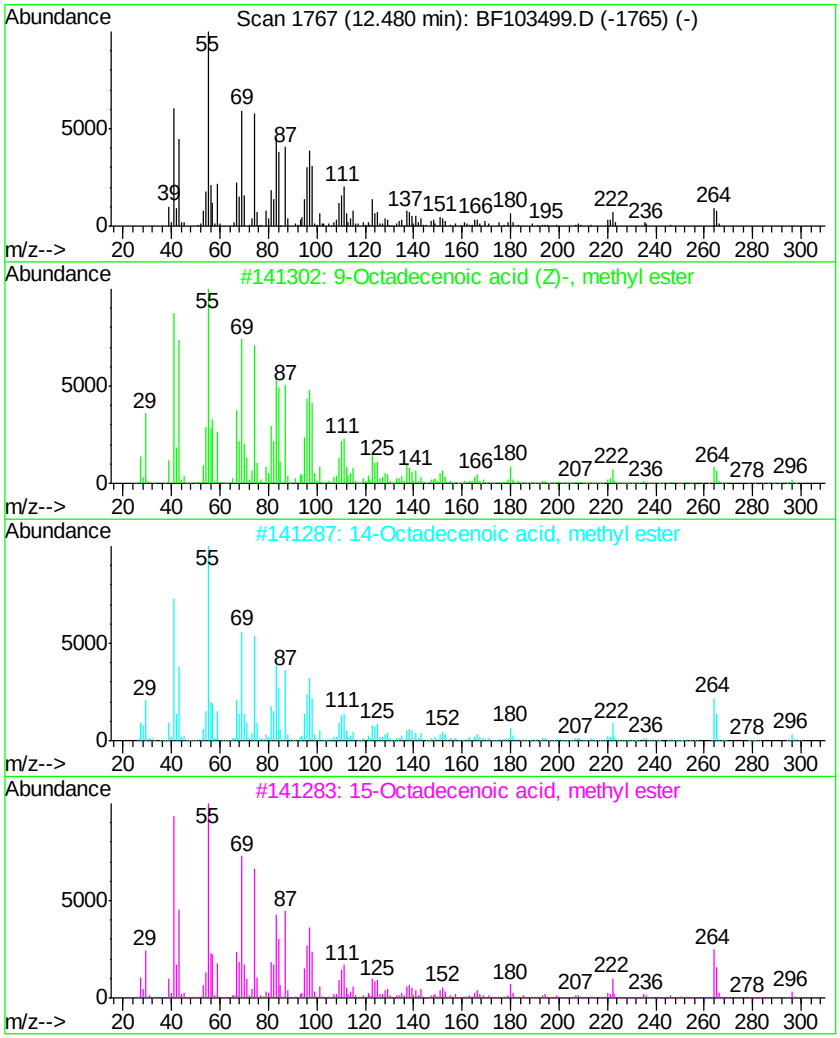
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

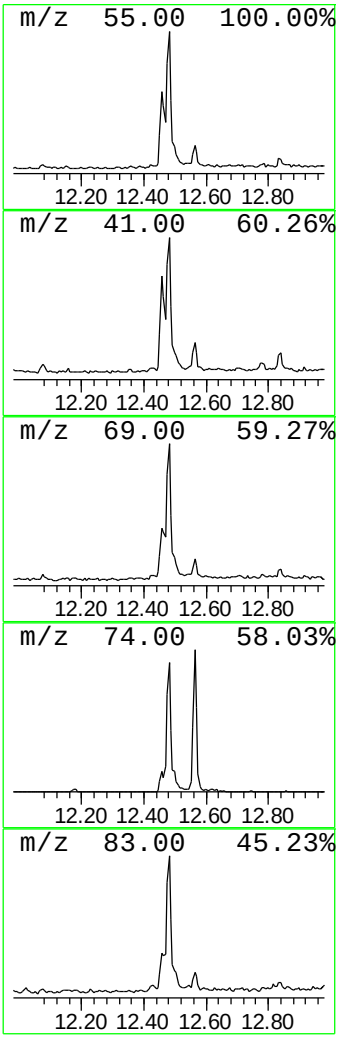
****

Peak Number 8 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	12.33 ng	686726	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
3	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	91
4	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	91
5	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91





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Data File : BF103499.D
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Operator : SJ/JU
Sample : J1699-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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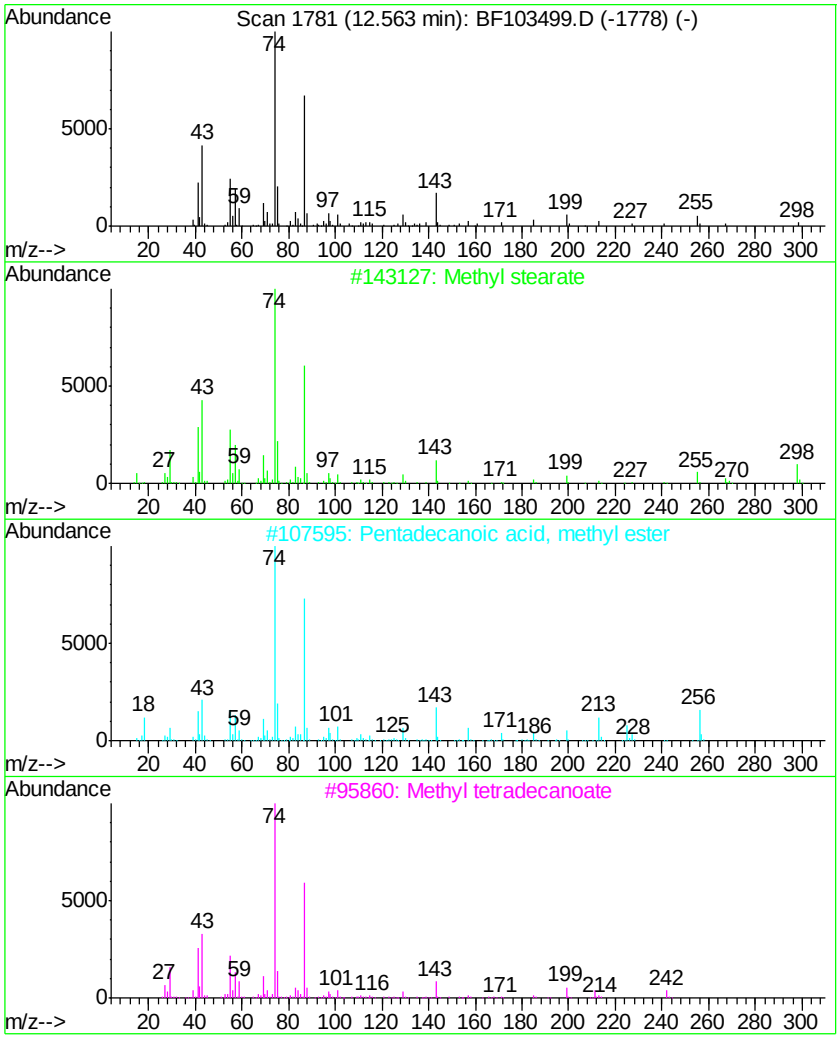
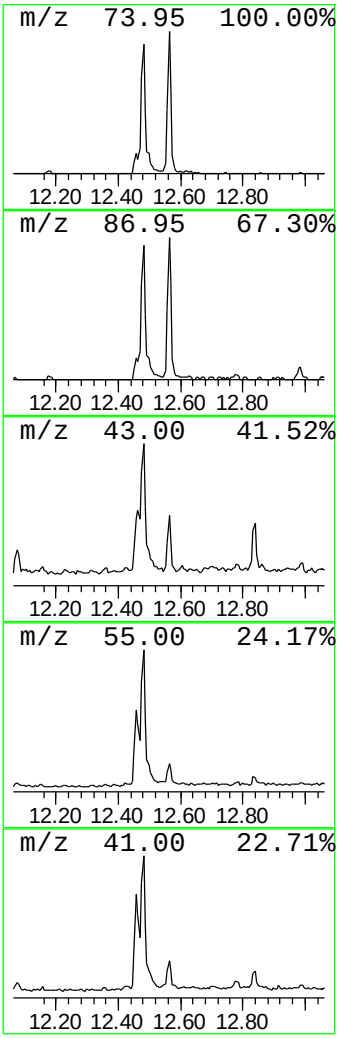
Peak Number 9 Methyl stearate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	2.52 ng	140548	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl stearate	298	C19H38O2	000112-61-8	97
2	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	94
3	Methyl tetradecanoate	242	C15H30O2	000124-10-7	91
4	Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	91
5	Hexadecanoic acid, 15-methyl-, m...	284	C18H36O2	006929-04-0	91





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Sample : J1699-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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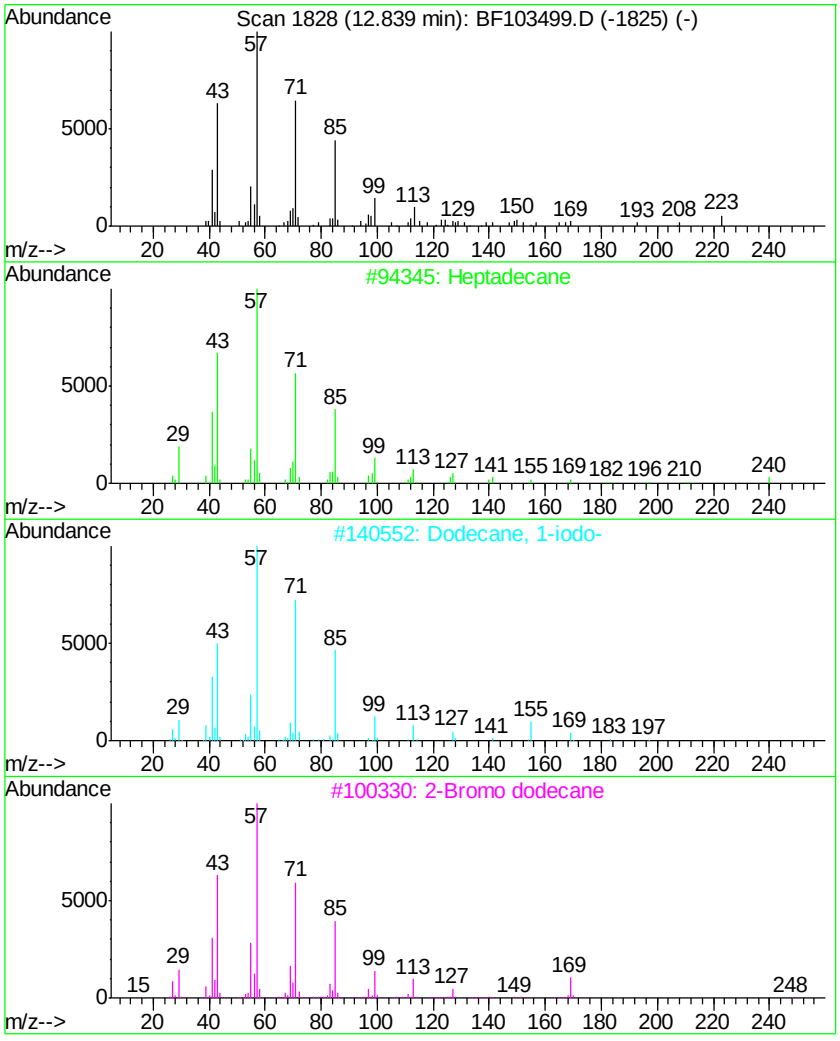
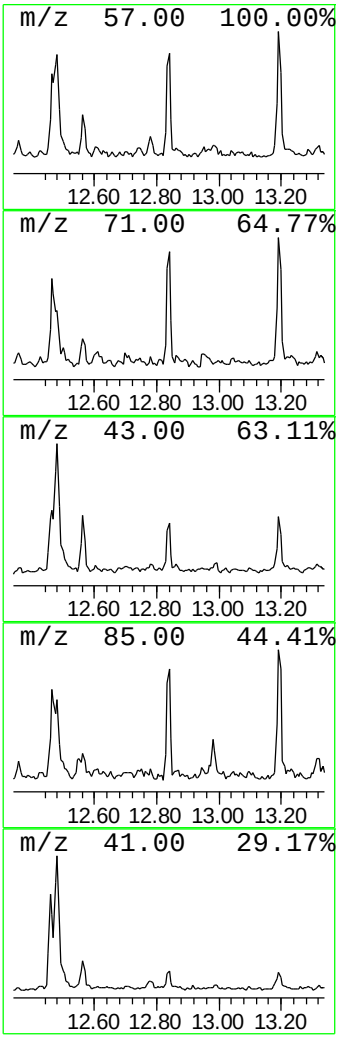
Peak Number 10 Heptadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.84	2.16 ng	78268	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	83
2	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	78
4	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	72





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030718\
Data File : BF103499.D
Acq On : 7 Mar 2018 14:28
Operator : SJ/JU
Sample : J1699-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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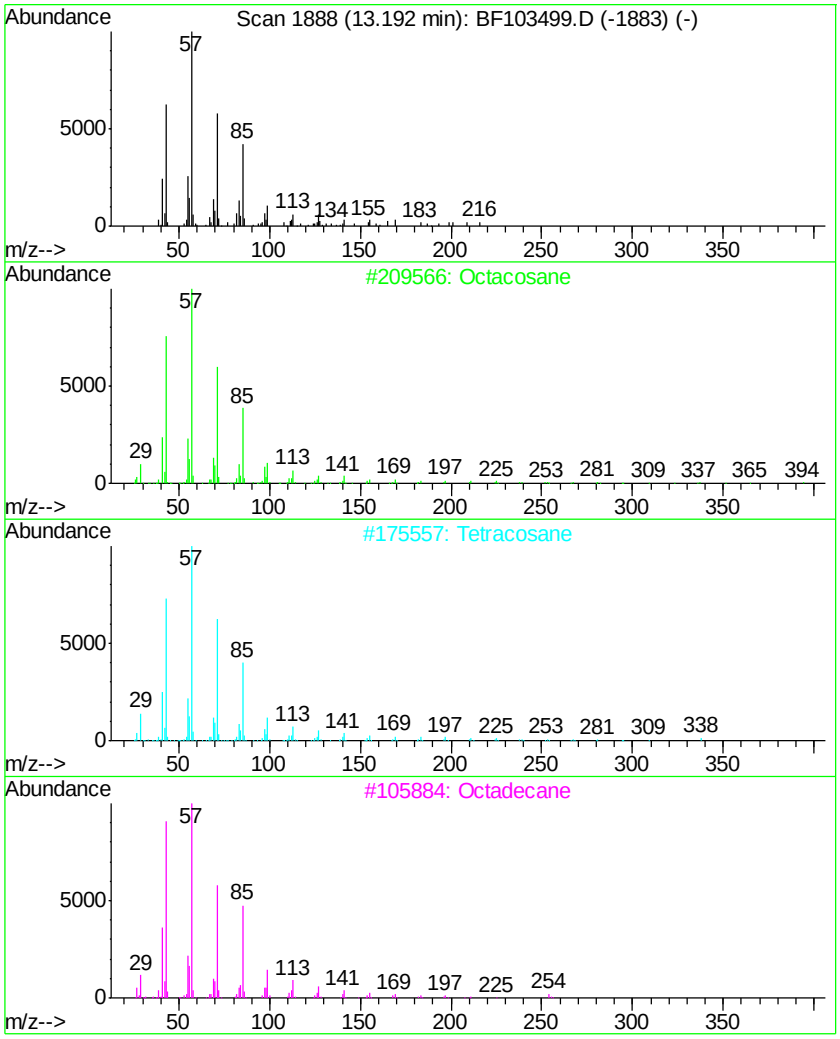
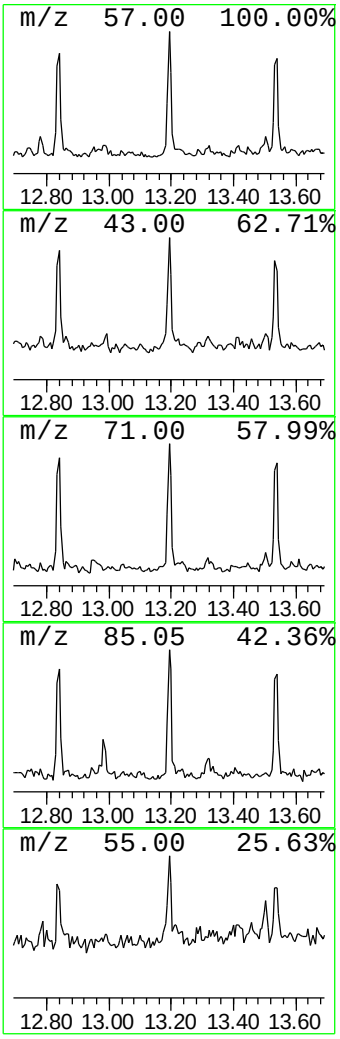
Peak Number 11 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.19	2.80 ng	101355	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Octadecane	254	C18H38	000593-45-3	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Heneicosane	296	C21H44	000629-94-7	91





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Data File : BF103499.D
Acq On : 7 Mar 2018 14:28
Operator : SJ/JU
Sample : J1699-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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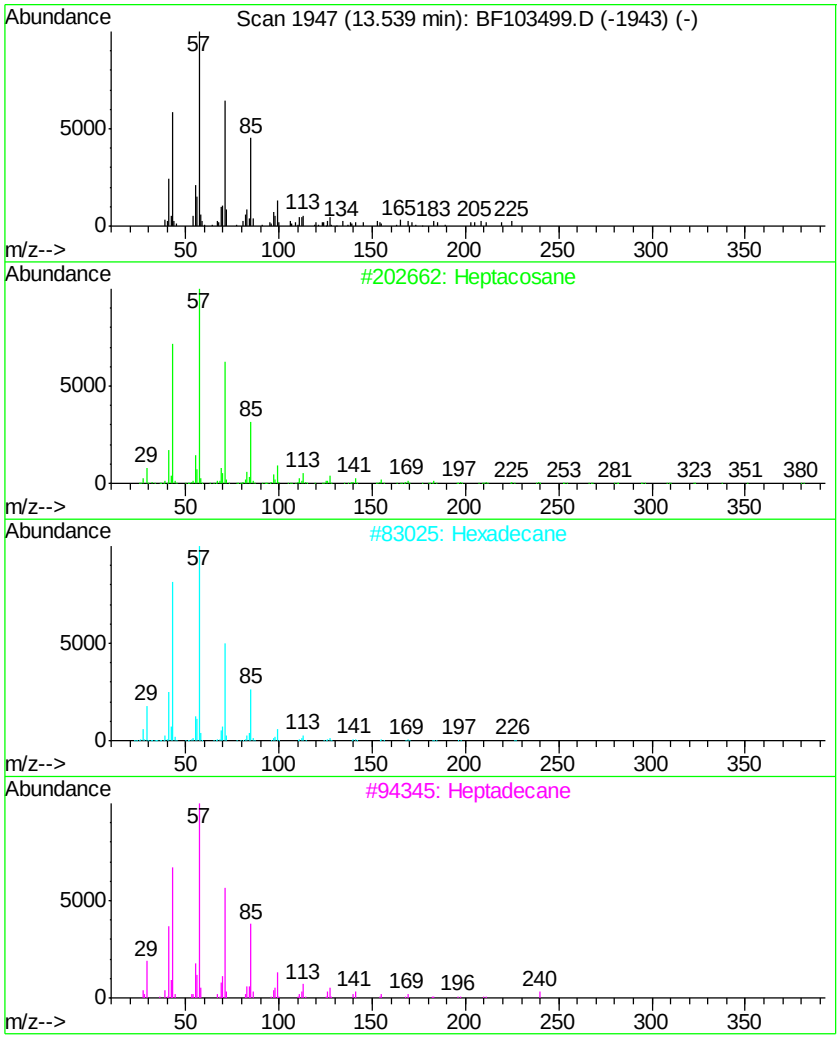
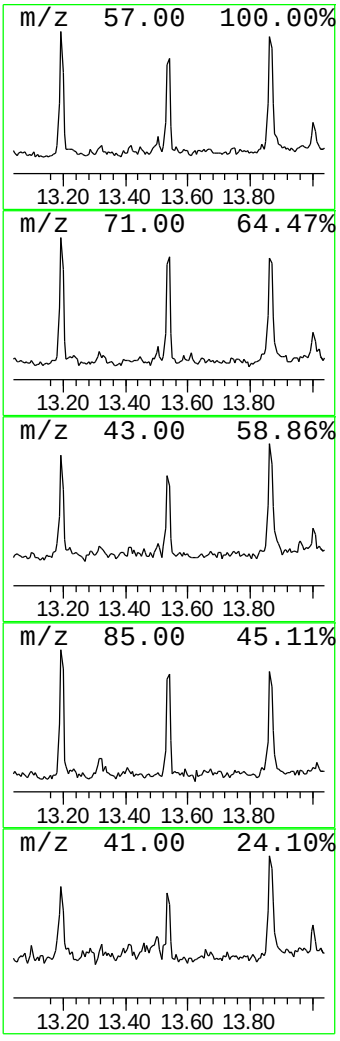
Peak Number 12 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.54	2.28 ng	82643	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Hexadecane	226	C16H34	000544-76-3	83
3	Heptadecane	240	C17H36	000629-78-7	72
4	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	64
5	Bacchotricuneatin c	342	C20H22O5	066563-30-2	62





Data Path : Z:\HPCHEM1\BNA F\DATA\BF030718\
Data File : BF103499.D
Acq On : 7 Mar 2018 14:28
Operator : SJ/JU
Sample : J1699-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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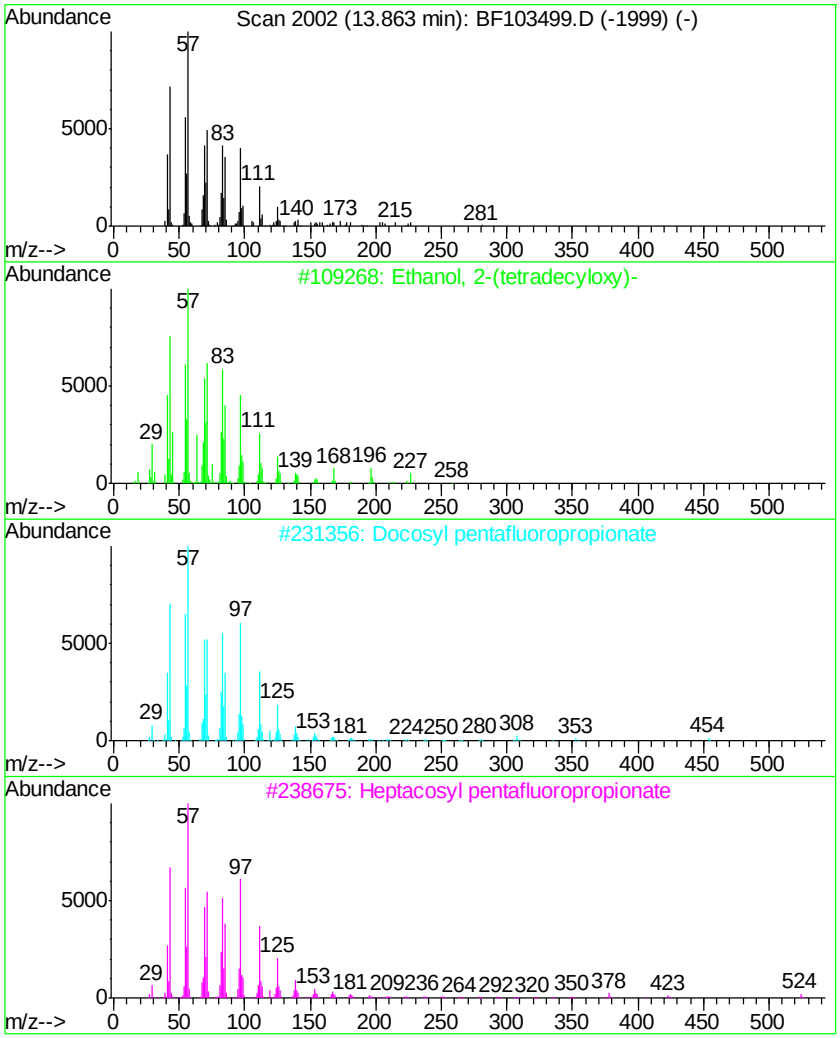
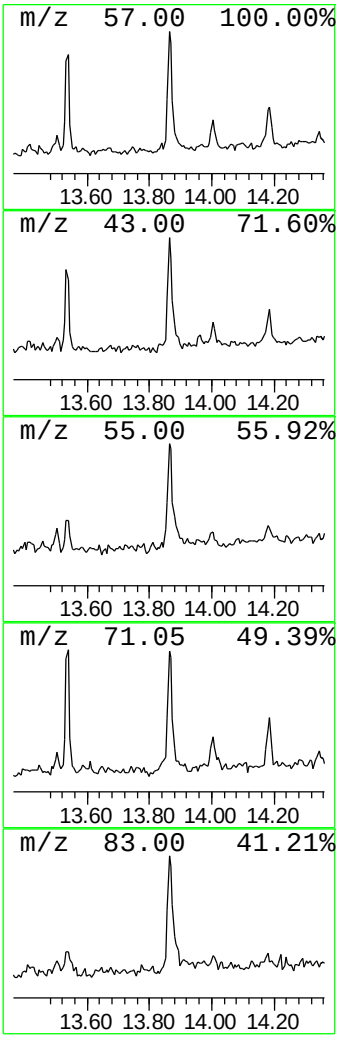
Peak Number 13 Ethanol, 2-(tetradecyloxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	4.54 ng	164218	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
2	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
3	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	91
4	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	91
5	Hexacosyl pentafluoropropionate	528	C29H53F5O2	1000351-81-2	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030718\
Data File : BF103499.D
Acq On : 7 Mar 2018 14:28
Operator : SJ/JU
Sample : J1699-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : B5

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF022218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.14	7.3	ng	315701	1	6.86	868449	20.0
2-Pentanone, 4-hy...	5.10	2.1	ng	89247	1	6.86	868449	20.0
unknown6.63	6.63	66.8	ng	2899790	1	6.86	868449	20.0
2,2,4-Trimethyl-1...	9.09	2.8	ng	171581	3	9.90	1211510	20.0
Hexadecanoic acid...	11.77	4.1	ng	230511	4	11.40	1114220	20.0
9,12-Octadecadien...	12.46	8.4	ng	466401	4	11.40	1114220	20.0
9-Octadecenoic ac...	12.48	12.3	ng	686726	4	11.40	1114220	20.0
Methyl stearate	12.56	2.5	ng	140548	4	11.40	1114220	20.0
Heptadecane	12.84	2.2	ng	78268	5	14.06	723593	20.0
Octacosane	13.19	2.8	ng	101355	5	14.06	723593	20.0
Heptacosane	13.54	2.3	ng	82643	5	14.06	723593	20.0
Ethanol, 2-(tetra...	13.86	4.5	ng	164218	5	14.06	723593	20.0